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Gauss quadrature generated by diagonalization of H in finite L^2 bases

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Using the J matrix method, diagonalization of $H_0 + V$ in certain finite L^2 basis sets is shown to generate a Gauss quadrature of the continuum. Explicit formulas for the corresponding weight function and orthogonal polynomials are given. This leads to a particularly simple expression for the Fredholm determinant and to the equivalence of the J matrix and Fredholm equivalent-quadrature methods. Consideration of the asymptotic behavior of the polynomials for large degree results in a proof of Heller's derivative rule relating the spacing of pseudostate eigenvalues to the relative normalization of pseudostate and continuum matrix elements, and providing an alternative to Stieltjes imaging for the solution of the classical moment problem. Applications include an accurate quadrature of the sum over a complete set of intermediate states in perturbation expansions.

I. INTRODUCTION

The calculation of the wave function and cross section for scattering from a potential or a complex target generally presents a more demanding task than the determination of a single bound state. Not only do the boundary conditions at large separation lead to eigenfunctions normalizable only in the sense of a δ functional, but one usually also desires results at a whole range of energies. Nevertheless, new methods have recently been introduced which employ the diagonalization of the Hamiltonian in a finite L^2 basis as the major computational step just as for the determination of a set of bound states, and then extract a good approximation to the continuum solution by imposing appropriate boundary conditions.[1-13]

Qualitatively how continuum information is contained in an N-dimensional L^2 basis set representation of the Hamiltonian becomes clear on considering the location of the eigenvalues. If the basis set describes the interaction well, the lowest few eigenvalues usually correspond closely to the exact bound states, but the higher roots lie less close to the higher-energy bound states and several of the eigenvalues appear at positive energies in what should be the continuum. Many workers have used these higher-lying pseudostates[14] in configuration interaction calculations in an attempt to introduce an average effect of the spectral density of the higher bound states and continuum. Heller *et al.*[8], made this idea more precise by suggesting that the diagonalization of H in an N term L^2 basis generates a Gauss quadrature[15] of the spectral density with the positive pseudostate eigenvalues directly related to the quadrature abscissas and the change from continuum δ functional to discrete Kronecker δ normalization to the weights and the weight function. Further work[8,10] showed that in certain special L^2 basis sets the radial kinetic energy operator H_0 is tridiagonal, causing its eigenvalues in the first N basis functions to be directly related to the zeros of well-known orthogonal polynomials of degree N, and hence at the abscissas of the corresponding Gauss quadrature. Armed with explicit knowledge of the quadrature generated by the diagonalization of H_0 and by careful handling of the singularity in the spectral resolution of the free Green's function $(H_0 - E)^{-1}$, Heller, *et al.*[9] were able to obtain a good numerical approximation to continuum properties with a finite L^2 basis. We discuss the quadrature suggestion and review their work in Sec. II.

At the same time, Heller and Yamani[2] learned of another way to exploit the tridiagonal structure of H_0 in the special basis sets. By truncating the representation of the potential to the first N basis functions and maintaining an infinite set for H_0, they were able to solve the Schrödinger equation exactly for the approximate potential with one major computational step involving the diagonalization of the full Hamiltonian as a matrix in the first N basis functions. The results of the J-matrix method for potential scattering needed here are given in Sec. III.

In Sec. IV, we use the J-matrix method to find the Gauss quadrature generated by diagonalizing the full Hamiltonian in the same basis sets in which H_0 is tridiagonal. A comparison of the quadrature approximations to the spectral resolution of the full Green's function and of the identity with the J-matrix results reveals the explicit form of the weight function and orthogonal polynomials which characterize the quadrature. To avoid difficulties encountered by Yamani and Reinhardt[10] with the attractive Coulomb potential, we restrict the analysis to potentials too weakly attractive to

bind and defer the extension to stronger potentials to a subsequent paper.

In Sec. V, we use the explicit form of the quadrature to investigate the dispersion integral of the Fredholm determinant,[16] or Jost function, resulting in an impressively simple relation between the quadrature weight function and the spectral density. Continuing in Sec. VI, we use the large degree asymptotic behavior of the orthogonal polynomials to prove a conjecture by Heller[7,10] relating the spacing of the pseudostate eigenvalues to the relative normalization of the pseudostate and actual continuum matrix elements. This provides an alternative to Stieltjes[11] imaging for the solution of the classical moment problem as well as an interesting formula for the scattering phase shift in terms of the relative spacing of the eigenvalues of H_0+V and H_0 alone.

The simplicity of the results of Secs. IV–VI leads us to conjecture in Sec. VII that the quadrature idea is valid for arbitrary finite L^2 basis sets. In addition, the extensions to potentials with bound states and to multichannel scattering are outlined and an accurate quadrature of perturbation sums over complete sets of intermediate states is discussed.

II. EQUIVALENT QUADRATURE

A. Introduction. Review of Gauss quadrature

A Gauss quadrature can be developed from a weight function $\rho(x)$, positive on the desired integration interval (a,b) with the help of the polynomials orthogonal with respect to ρ,[15]

$$\int_a^b dx\, p_n(x)\, p_m(x)\rho(x) = h_n \delta_{nm} . \tag{2.1}$$

For an arbitrary $\rho(x)$, p_n can be generated by Gram-Schmidt orthogonalization of the first $n+1$ algebraic moments. In most cases, it is more efficient, however, to employ the three term recursion relation

$$p_{n+1}(x) = (A_n x + B_n) p_n(x) + C_n p_{n-1}(x) , \tag{2.2}$$

starting with $p_{-1}=0$ and $p_0=1$, which follows from the polynomial character and the orthogonality relation (2.1). The best quadrature of degree n of the integral of $\rho(x)$ with a function $f(x)$ then takes the form:

$$\int_a^b dx\, \rho(x) f(x) = \sum_{i=1}^{n} w_i^n f(x_i^{(n)}), \tag{2.3}$$

where the abscissas are given by $p_n(x_i^{(n)})=0$, and the weights by the Christoffel formula:

$$w_i^n = A_{n-1} h_{n-1} [p_{n-1}(x_i^{(n)}) p_n'(x_i^{(n)})] , \tag{2.4}$$

with p_n' indicating differentiation with respect to x. It is straightforward to show that the $2n$ pieces of information in the w_i and x_i suffice to integrate a polynomial of degree $\leq 2n-1$ exactly.

B. Idea of an equivalent quadrature

Since diagonalizing a Hamilton operator in a finite L^2 basis requires determining the roots of the secular determinant, a polynomial in E, it is not surprising that there should be some relation between the pseudostate eigenvalues and the abscissas of a Gauss quadrature of the continuous spectrum. Heller and co-workers[8,10] discovered the correct relation for certain special cases by comparing the matrix elements of an operator in a finite L^2 basis with a quadrature of the exact continuum elements. We will follow their approach in examining the spectral representation of the Green's function $(H-E)^{-1}$.

If H has no bound states, matrix elements of the real part of the Green's function between two square integrable states $|i\rangle$ and $|f\rangle$ can be written as the principal value integral

$$\langle i | \mathcal{G}^P(E) | f \rangle = P \int_0^\infty dE' \, \frac{\langle i | E' \rangle \langle E' | f \rangle}{E' - E} . \tag{2.5}$$

When H is strong enough to bind, a sum over bound states must be added, but because of difficulties discussed below we will not complete this extension here.

By introducing a weight function ρ in some appropriate variable $x(E)$ and taking care to separate off the singularity at $E'=E$, Eq. (2.5) becomes

$$\begin{aligned}\langle i | \mathcal{G}^P(E) | f \rangle = & \int_{x(0)}^{x(\infty)} dE' \, \rho(x') \frac{dx'}{dE'} \frac{\langle i | E' \rangle \langle E' | f \rangle}{\rho(x')(E'-E)} \\ & - \frac{\langle i | E \rangle \langle E | f \rangle}{\rho(x)(x'-x)} \\ & + \frac{\langle i | E \rangle \langle E | f \rangle}{\rho(x)} P \int_{x(0)}^{x(\infty)} \frac{dx' \rho(x')}{x'-x} ,\end{aligned} \tag{2.6}$$

allowing us to obtain a quadrature approximation of degree N in accordance with Eq. (2.3),

$$\begin{aligned}\langle i | \mathcal{G}^P(E) | f \rangle \simeq & \sum_j^N \frac{w_j}{\rho(x_j)} \left(\frac{dE'}{dx}\right)_{x_j} \frac{\langle i | E(x_j) \rangle \langle E(x_j) | f \rangle}{E(x_j) - E} \\ & + \frac{\langle i | E \rangle \langle E | f \rangle}{\rho(x)} \\ & \times \left(P \int_{x(0)}^{x(\infty)} \frac{dx' \rho(x')}{x'-x} - \sum_{j=1}^{N} \frac{w_j}{x_j - x} \right) .\end{aligned} \tag{2.7}$$

The first term resembles the elements of the matrix inverse of $H-E$, denoted by $\tilde{\mathcal{G}}(E)$, in an N term L^2 basis,

$$\langle i|\tilde{\mathcal{G}}(E)|f\rangle = \sum_{j=1}^{N} \frac{\langle i|\Psi_j\rangle\langle\Psi_j|f\rangle}{E_j - E}\ , \tag{2.8}$$

if $|\Psi_j\rangle$ is the pseudostate, or normalized discrete L^2 eigenvector of positive energy E_j. Heller, and co-workers[8,10] went further to propose that if a weight function ρ in a variable x can be found such that the energy at each abscissa $E(x_j)$ equals the pseudostate energy E_j, then the first term in Eq. (2.7) can be equated to Eq. (2.8). The reason for the additional factors in the sum in Eq. (2.7) is apparent on realizing that the pseodostates $|\Psi_j\rangle$ are normalized to a Kronecker δ while the continuum functions evaluated at the energy E_j are normalized to a Dirac δ function in E.[16] Thus, solving for a continuum matrix element yields

$$|\langle i|E_j\rangle \simeq \left(\frac{\rho(x_j)}{w_j}\left(\frac{dx}{dE}\right)_{x_j}\right)^{1/2} |\langle i|\Psi_j\rangle|\ . \tag{2.9}$$

We note that for Eq. (2.9) to be a good approximation, the L^2 state $|i\rangle$ must be well described by the N-dimensional L^2 basis. In addition, the nonsquare integrable continuum function $|E_j\rangle$ is only represented by the pseudostate $|\Psi_j\rangle$ in the sense of a distribution, i.e., as part of a scalar product with an L^2 function such as $|i\rangle$.

For certain special cases, Yamani and Reinhardt[10] were able to verify Eq. (2.9) explicitly. When the kinetic energy operator

$$H_0 = -\frac{1}{2}\frac{d^2}{dr^2} + \frac{l(l+1)}{2r^2} \tag{2.10}$$

is diagonalized in the nonorthogonal Slater basis

$$\phi_n = (\lambda r)^{l+1} e^{-\lambda r/2} L_n^{2l+1}(\lambda r),\quad n = 0, 1, \ldots, N-1 \tag{2.11}$$

(where L_n^{2l+1} is a Laguerre polynomial[15] and λ a scale parameter) the eigenvalues are related to the zeros of the Gegenbauer polynomials[15] $C_n^{l+1}(x)$, which are orthogonal with respect to the weight function $(1-x^2)^{l+1/2}$ on $x\in(-1,1)$, by

$$E_j = E(x_j);\quad E(x) = \tfrac{1}{8}\lambda^2(1+x)/(1-x)\ . \tag{2.12}$$

In addition, they found a similar correspondence in the oscillator basis

$$\phi_n = (\lambda r)^{l+1} e^{-\lambda^2 r^2/2} L_n^{l+1/2}(\lambda^2 r^2) \tag{2.13}$$

between the eigenvalues of the kinetic energy and the zeros of the Laguerre polynomials, $L_n^{l+1/2}$, orthogonal with respect to $x^{l+1/2}e^{-x}$ on $x\in(0,\infty)$, and where $x = 2E/\lambda^2$. Given the weight function and polynomials, they were able to prove Eq. (2.9) and perform the principle value integral in Eq. (2.7).

In investigating the addition of a Coulomb potential to Eq. (2.10), they found that the operator

$$H_0 = -\frac{1}{2}\frac{d^2}{dr^2} + \frac{l(l+1)}{2r^2} + \frac{z}{r} \tag{2.14}$$

is tridiagonal only in the basis (2.11),[10] and for $z>0$ the eigenvalues are displaced to correspond to the zeros of the relatively recently introduced Pollaczek polynomials, $p_n^{l+1}(2z/\lambda, -2z/\lambda, x)$,[15,17] orthogonal with respect to the weight function

$$\rho(x) = \frac{2^{2l+1}(1-x^2)^{l+1/2}|\Gamma(l+1-iz/k)|^2}{\pi\exp[(2\theta-\pi)z/k]}\ , \tag{2.15}$$

where $\theta = \cos^{-1}(x)$, k is the momentum and $x\in(-1,1)$ and is related to E by Eq. (2.12). While using negative values of z does not disturb the eigenvalue correspondence in Eq. (2.12), the weight function (2.15) must then be extended to negative energies, where it takes the form of a jump function rising abruptly at each of the Coulomb bound states where $\Gamma(l+1-iz/k)$ has poles.[10] Because it is not clear how to establish the orthogonality of the polynomials on this extended weight function and how to represent the infinite Rydberg series by the bound pseudostates, we limit the discussion here to $z\geq 0$ and to potentials too weakly attractive to bind in general.

III. J-MATRIX THEORY OF POTENTIAL SCATTERING: RESULTS

The J-matrix theory[2-7] exploits the tridiagonal form of H_0 by constructing the coefficients for the expansion of two independent solutions of the H_0 Schrödinger equation in the bases (2.11) and (2.13). First a regular solution,

$$S(kr) = \sum_{n=0}^{\infty} s_n(x)\phi_n(r)\ , \tag{3.1}$$

identical to the spherical Riccati Bessel function[16] for $z=0$, or the regular Coulomb wave for $z\neq 0$, is formed by requiring

$$\langle\phi_n|H_0 - E|S(k,r)\rangle = \sum_{n'=0}^{\infty} J_{nn'}s_{n'} = 0\ ,$$
$$n = 0, 1, 2\ldots, \tag{3.2}$$

where

$$J_{nn'} \equiv \langle\phi_n|H_0 - E|\phi_{n'}\rangle. \tag{3.3}$$

(Since the angular momentum is held fixed throughout the discussion, an indexing of each function with l is suppressed.)

Since the matrix J is of Jacobi, or tridiagonal form, Eq. (3.2) amounts to a three term recursion relation for the s_n, related to that for the polynomials mentioned in Sec. II, which we desig-

nate as

$$p_n^0 = k_n^0 \sum_{j=1}^{n} (x - {}^0x_j^n) , \tag{3.4}$$

orthogonal on a weight function ρ_0 in a variable x conformally mapped from the energy so that

$$\int_{x(0)}^{x(\infty)} dx\, \rho_0(x) p_n^0(x) p_n^0(x) = h_n^0 \delta_{nn} , \tag{3.5}$$

yielding

$$s_n(x) = a_n [X^{1/2}(x)\rho_0(x)]^{1/2} p_n^0(x) . \tag{3.6}$$

The particular results for zero or nonzero z and the Slater and oscillator bases are summarized in Table I. Rather than choosing the second, independent function

$$C(k,r) = \sum_{n=0}^{\infty} c_n(x)\phi_n(r) \tag{3.7}$$

to be identical with the respective irregular solution of the Schrödinger equation, which would make the expansion in the inherently regular basis functions ill behaved, the coefficients c_n are chosen to obey an inhomogeneous version of the recursion relation (3.2):

$$\sum_{n'=0}^{\infty} J_{nn'} c_{n'} = \frac{k}{2} \frac{\delta_{n0}}{s_0} . \tag{3.8}$$

The solution $C(r)$ is then regular at the origin, but still has the same asymptotic behavior as the irregular solution for large r. Although explicit, readily calculable, formulas for the c_n for each case are derived in Ref. 3, it is useful to cast them in a new form as

$$c_n = a_n [X^{1/2}(x)\rho_0(x)]^{1/2} q_n^0(x) , \tag{3.9}$$

where q_n^0 is a function conjugate to p_n^0 defined by the principle value integral

$$q_n^0(x) \equiv \frac{P}{\pi\rho_0(x)} \int_{x(0)}^{x(\infty)} \frac{dx' \rho_0(x') p_n^0(x')}{x' - x} . \tag{3.10}$$

By subtracting off and readding the avoided singularity at $x' = x$, q_n^0 can be expressed in terms of the Gauss quadrature belonging to ρ_0 (Ref. 15)

TABLE I. J-matrix method results (Refs. 2 and 3) for the expansion of free and Coulomb waves in certain L^2 basis sets. In the oscillator and Slater L^2 basis sets given, the overlap matrix ($s_{nn'}$) and $J = (H_0 - E)$ matrix are symmetric tridiagonal. This allows analytic determination of the expansion coefficients $a_n p_n^0(x)$ of the free wave function in each basis, with p_n^0 the polynomial of degree n in $x(E)$ of the set orthogonal with respect to the weight function ρ_0 with normalization constant h_n^0 and coefficient of x^n k_n^0. In the Slater basis, the results were extended to the Coulomb wave function for charge z.

Basis set	Oscillator	Slater	
$\phi_n(r)$	$(\lambda r)^{l+1} e^{-\lambda^2 r^2/2} L_n^{l+1/2}(\lambda^2 r^2)$	$(\lambda r)^{l+1} e^{-\lambda r/2} L_n^{2l+1}(\lambda r)$	
$s_{nn'}$	$\frac{\delta_{nn'}\Gamma(n+l+3/2)}{2\lambda\Gamma(n+1)}$	$\frac{\Gamma(n+2l+2)}{\lambda\Gamma(n+1)}\left[2(n+l+1)\delta_{nn'} - n\delta_{n-1,n'} - (n+2l+2)\delta_{n+1,n'}\right]$	
J_{nn}	$\frac{\lambda\Gamma(n+l+3/2)(2n+l+3/2-x)}{4\Gamma(n+1)}$	$\frac{-\lambda\Gamma(n+2l+2)}{2(1-x)\Gamma(n+1)}\left[x(n+l+1) - z/k \sin\theta\right]$; where $x = \cos\theta$	
$J_{n,n-1}$	$\frac{\lambda\Gamma(n+l+3/2)}{4\Gamma(n)}$	$\frac{\lambda\Gamma(n+2l+2)}{4(1-x)\Gamma(n)}$	
$x(E)$	$2E/\lambda^2$	$(E - \lambda^2/8)/(E + \lambda^2/8)$	
$X(x)$	x	$1 - x^2$	
Charge	0	0	z
ρ_0	$e^{-x} x^{l+1/2}$	$(\sin\theta)^{2l+1}$	$\frac{(2\sin\theta)^{2l+1}\lvert\Gamma(l+1-iz/k)\rvert^2}{\pi\exp\{2\theta - \pi)z/k\}}$
Polynomial	Laguerre	Gegenbauer	Pollaczek
p_n^0	$L_n^{l+1/2}$	C_n^{l+1}	$P_n^{l+1}(x; 2z/\lambda, 2z/\lambda)$
a_n	$\frac{(-1)^n(2\pi)^{1/2}\Gamma(n+1)}{\Gamma(n+l+3/2)}$	$\frac{2^l\Gamma(l+1)\Gamma(n+1)}{\Gamma(n+2l+2)}$	$\frac{(\pi/2)^{1/2}\Gamma(n+1)}{\Gamma(n+2l+2)}$
h_n^0	$\frac{\Gamma(n+l+3/2)}{\Gamma(n+1)}$	$\frac{\pi\Gamma(n+2l+2)}{2(n+l+1)\Gamma(n+1)2^{2l}\Gamma^2(l+1)}$	$\frac{\Gamma(n+2l+2)}{(n+l+1+2z/\lambda)\Gamma(n+1)}$
k_n^0	$\frac{(-1)^n}{\Gamma(n+1)}$	$\frac{2^n\Gamma(n+l+1)}{\Gamma(n+1)\Gamma(l+1)}$	$\frac{2^n\Gamma(n+l+1+2z/\lambda)}{\Gamma(n+1)\Gamma(l+1+2z/\lambda)}$

$$q_n^0(x)=\frac{1}{\pi\rho_0(x)}\int_{x(0)}^{x(\infty)}dx'\,\rho_0(x')\frac{p_n^0(x')-p_n^0(x)}{x'-x}+\frac{p_n^0(x)P}{\pi\rho_0(x)}\int_{x(0)}^{x(\infty)}\frac{dx'\,\rho_0(x')}{x'-x}$$

$$=\frac{p_n^0(x)}{\pi\rho_0(x)}\left(P\int_{x(0)}^{x(\infty)}\frac{dx'\,\rho(x')}{x'-x}-\sum_{j=1}^{n}\frac{{}^0w_j^n}{{}^0x_j^n-x}\right), \tag{3.11}$$

where

$$p_n^0({}^0x_j^n)=0 \quad \text{for } j=1,2,\ldots,n\ .$$

The quadrature of the nonsingular integral above is exact, since the integrand contains ρ_0 times a polynomial of degree less than $2n$.[15] This form for the q_n^0 will prove useful in conjunction with the dispersion correction term in Eq. (2.7).

Given the s_n and c_n, the standing wave, or principal value, wave function for scattering by a potential can be expanded in the basis set (2.11) or (2.13),

$$\Psi^P(k,r)=\sum_{n=0}^{\infty}R_n(x)\phi_n(r)\ . \tag{3.12}$$

By approximating the potential through a truncation of the basis set expansion to N terms

$$V_{\text{app}}=\sum_{n=0}^{N=1}\sum_{n'=0}^{N=1}|\,\bar{\phi}_n\rangle\langle\,\phi_n|\,V|\,\phi_{n'}\rangle\langle\bar{\phi}_{n'}|\,, \tag{3.13}$$

where $\bar{\phi}_n$ is biothogonal to ϕ_n such that

$$\langle\,\bar{\phi}_n|\,\phi_{n'}\rangle=\delta_{nn'}, \tag{3.14a}$$

where

$$\langle\,\phi_n|\,\phi_{n'}\rangle=s_{nn'}, \tag{3.14b}$$

the coefficients R_n can be determined exactly for the approximate potential by requiring

$$\sum_{m'=0}^{\infty}(H_0+V_{\text{app}}-E)_{mm'}R_{m'}(x)=0, \quad m=0,1,2,\ldots\ . \tag{3.15}$$

The result is

$$R_n(x)=s_n+\tan\delta c_n \quad \text{for } n\geq N-1\ , \tag{3.16a}$$

$$R_n(x)=-\tilde{\mathcal{G}}_{n,N-1}(E)J_{N-1,N}R_N(x) \quad \text{for } n\leq N-1, \tag{3.16b}$$

with

$$\tilde{\mathcal{G}}_{nn'}=\sum_{j=1}^{N}\frac{\Gamma_{nj}\Gamma_{n'j'}}{E_j-E}\ , \tag{3.17}$$

an element of the inverse of the $N\times N$ matrix of $H_0+V_{\text{app}}-E$ expressed in terms of the matrix of eigenvectors Γ_{nj} and the eigenvalues E_j obtained from the diagonalization of H_0+V_{app} in the first N basis functions. The tangent of the phase shifts is given as

$$\tan\delta(E)=-\frac{\tilde{\mathcal{G}}_{N-1,N-1}J_{N-1,N}s_N+s_{N-1}}{\tilde{\mathcal{G}}_{N-1,N-1}J_{N-1,N}c_N+c_{N-1}} \tag{3.18}$$

(see Table I for $J_{N-1,N}$ for each case). Combining the recursion relation for s_n and c_n (3.2 and 3.8) with Eqs. (3.16a) and (3.18) yields a simplified expression for R_N,

$$R_N(x)=-k/[2(\tilde{\mathcal{G}}_{N-1,N-1}J_{N-1,N}c_N+c_{N-1})J_{N-1,N}]\,. \tag{3.19}$$

From Eq. (3.17) it is clear that

$$R_N(x_j)=0 \quad \text{for } j=1,2,\ldots,N, \tag{3.20}$$

where

$$x_j\equiv x(E_j)\ , \tag{3.21}$$

which is suggestive of the location of the abscissas of a Gauss quadrature at the energy eigenvalues. In order to construct the matrix elements of the full Green's function, Heller[4] introduced a second function, independent of Ψ^P,

$$I(k,r)=\sum_{n=0}^{\infty}I_n(x)\phi_n(r)\ , \tag{3.22}$$

analogous to $C(k,r)$ of Eq. (3.7), which is regular at the origin but approaches the irregular solution of the Schrödinger equation with the truncated potential at large r. Similar to Eq. (3.8) for the c_n, the I_n obey the recursion relation

$$\sum_{n'}(H_0+V_{\text{app}}-E)_{nn'}I_{n'}=\frac{k(1+\tan^2\delta)\,\delta_{n0}}{2R_0}\ , \tag{3.23}$$

and are given by

$$I_n=c_n-\tan\delta s_n \quad \text{for } n\geq N-1\ , \tag{3.24a}$$

$$I_n=-\tilde{\mathcal{G}}_{n,N-1}J_{N-1,N}I_N+[k(1+\tan^2\delta)/2R_0]\tilde{\mathcal{G}}_{n0}\ . \tag{3.24b}$$

The matrix elements of the full Green's function can then be written as

$$\mathcal{G}^{\pm}_{nn'}=\lim_{\epsilon\to 0}\langle\,\bar{\phi}_n|\,[H_0+V_{\text{app}}-(E\pm i\epsilon)]^{-1}|\,\bar{\phi}_{n'}\rangle$$

$$=\mathcal{G}^{P}_{nn'}\pm 2i\,R_nR_{n'}/[k(1+\tan^2\delta)] \tag{3.25a}$$

where

$$\mathcal{S}^{P}_{nn'} = \begin{cases} 2R_n \langle I_n \rangle / [k(1+\tan^2\delta)] & \text{for } n_> \geq N-1 \\ \tilde{\mathcal{S}}_{nn'} + 2R_n R_{n'} I_N / [R_N k(1+\tan^2\delta)] & \text{for } n_> \leq N-1 \,. \end{cases} \tag{3.25b}$$

The J-matrix method owes its computational efficiency to the ability to perform the hardest part of the calculation, the determination of the matrix Γ_{nj} and eigenvalues E_j in Eq. (3.17), before choosing an energy, with relatively little effort required to complete the formation of the wave function and tangent of the phase shift at each energy. Evidently all the physics of the potential, that is the dynamics, is contained in Γ_{nj} and E_j, while the remaining factors of s_n and c_n only insure the asymptotic form appropriate to H_0, that is, the kinematics. In what follows we, above all, will exploit the exactness of Eqs. (3.16), (3.18), and (3.25) for scattering by the truncated potential (3.13).

IV. QUADRATURE GENERATED BY $H_0 + V_{app}$

A. Introduction

Equations (3.20) and (3.21) reveal a correspondence between the energy eigenvalues of $H_0 + V_{app}$ in an N-dimensional basis and the zeros of the Nth energy-dependent expansion coefficient R_N of the continuum wave function. This suggests a relation between $R_N(x)$ and a polynomial of degree N in x having the same zeros, in analogy to Eq. (3.6) for s_n in terms of the p_n^0. Following this suggestion in an analysis of the zeros of the other R_n immediately below and then of the spectral resolution of the identity and of the Green's function in Secs. IV B and IV C, we will characterize the quadrature generated by the diagonalization of $H_0 + V_{app}$ completely.

From the basis set form of the Schrödinger equation (3.15), we can extract the location of the zeros of $R_n(x)$ for $n \geq N-1$ as follows. Separating the sum over m' into two parts and considering only those components with $m \leq n-1$, Eq. (3.15) becomes

$$\sum_{m'=0}^{n-1} (H_0 + V_{app} - E)_{mm'} R_{m'}(x) = -\delta_{m,n-1} J_{n-1,n} R_n(x), \tag{4.1}$$

with the help of the tridiagonal form of $(H_0 + V_{app} - E)$ for m and $m' \geq N$ [see Eqs. (3.3) and (3.13)]. Thus at the zeros of $R_n(x)$

$$R_n(x_j^n) = 0 \tag{4.2}$$

for $j = 1, 2, \ldots, n$ and $n = N, N+1, \ldots$. Equation (4.1) is an eigenvalue equation,

$$\sum_{m'=0}^{n-1} (H_0 + V_{app} - E_j^n)_{mm'} R_{m'}(x_j^n) = 0 \tag{4.3}$$

for $m = 0, 1, \ldots, n-1$, with the eigenvalues of the $n \times n$ matrix $H_0 + V_{app} - E$ at

$$E_j^n = E(x_j^n) \tag{4.4}$$

for $j = 1, 2, \ldots, n$ and $n = N, N+1, \ldots$. This correspondence can be extended downward one more step by noting that for $n = N-1$ Eq. (4.1) becomes

$$\sum_{m=0}^{N-2} (H_0 + V_{app} - E)_{mm'} R_m(x) = -(H_0 + V_{app} - E)_{mN-1} \times R_{N-1}(x) \tag{4.1a}$$

for $m = 0, 1, \ldots, N-2$, and hence that Eqs. (4.2) and (4.4) also hold for $n = N-1$, but not for smaller n.

Now sure that the R_n have the desired zeros for $n \geq N-1$, we turn to the spectral resolution of the identity to find the corresponding polynomials and learn about the weight function with respect to which they are orthogonal.

B. Spectral resolution of the identity

The principle value, or standing wave functions, are complete when there are no bound states and are so normalized that[16]

$$\delta(r - r') = \frac{2}{\pi} \int_0^\infty \frac{dE \Psi^P(k,r) \Psi^P(k,r')}{k[1+\tan\delta(E)]} \,. \tag{4.5}$$

Taking the appropriate matrix element in the basis functions and using Eqs. (3.12) and (3.14) yields the orthogonality relation

$$\delta_{nn'} = \frac{2}{\pi} \sum_m \int_0^\infty dE \, \frac{R_n(x) R_m(x) s_{mn'}}{k[1+\tan^2\delta(E)]} \,. \tag{4.6}$$

For $n' \geq N$, this can be simplified considerably by noting that the R_m for $m \geq N-1$ in Eq. (3.16a) obey the recursion relation (3.2) and (3.8) for the s_n and c_n. Then, using the explicit forms of $s_{mn'}$ and $J_{mn'}$ given in Table I, it is straightforward to show that

$$\frac{2dE}{\pi k} \sum_m R_m s_{mn'} = \frac{dx\, R(x)}{X^{1/2}(x) a_{n'}^2 h_{n'}^0} \,, \tag{4.7}$$

and hence

$$\delta_{nn'} = \frac{1}{a_n a_{n'} h_n^0} \int_{x(0)}^{x(\infty)} \frac{dx\, R_n(x) R_{n'}(x)}{X^{1/2}(x)[1+\tan^2\delta(E)]} \tag{4.8}$$

where a_n, h_n^0, and $X(x)$ are given in Table I as well. This is to be compared with the orthogonality relation for the sought-after polynomials $p_n(x)$ on the

weight function[15] $\rho_{app}(x)$ generated from $H_0 + V_{app}$:

$$\delta_{nn'} = \frac{1}{h_n} \int_{x(0)}^{x(\infty)} dx\, \rho_{app}(x) p_n(x) p_{n'}(x) . \qquad (4.9)$$

Since, by Eq. (4.4), the zeros of $p_n(x)$ and $R_n(x)$ coincide, we are led from Eqs. (4.8) and (4.9) to

$$R_n(x) = a_n \{X^{1/2}(x)\rho_{app}(x) \times [1 + \tan^2\delta(E)]\}^{1/2} p_n(x) \text{ for } n \geq N , \qquad (4.10)$$

in close analogy to Eq. (3.6) for $s_n(x)$. Because as $E \to \infty$ $\Psi^P \sim S$ and $R_n \sim s_n$. choosing the constant a_n in Eq. (4.10) to be the same as in Eq. (3.6) normalizes the $p_n(x)$ to approach $p_n(x)$ as $E \to \infty$. Inserting Eq. (4.10) in (4.8) and comparing with Eq. (4.9) then yields $h_n = h_n^0$ for $n \geq N$. Since R_n and s_n obey the same recursion relation for $n \geq N$, the p_n obey the recursion relation for the p_n^0 for $n \geq N$, and can hence be written as

$$p_n(x) = k_n \prod_{j=1}^{n} (x - x_j^n) \text{ for } n \geq N , \qquad (4.11)$$

where k_n is determined by $p_n(x) \sim p_n^0$ as $E \to \infty$. In Appendix A, we verify that the ratio of $R_n(x)$ to $R_N(x)$ really is a polynomial of degree $n - N$ and that Eq. (4.10) holds for $n = N - 1$ as well.

Since the E_j are generated in solving the J-matrix equations, Eq. (4.10) can be used as an expression for the weight function in terms of known quantities.

$$\rho_{app}(x) = \frac{[R_N(x)/a_N p_N(x)]^2}{X^{1/2}(x)[1 + \tan^2\delta(E)]} . \qquad (4.10a)$$

With the weight function and polynomials of degree $n \geq N - 1$ determined, there remain only the polynomials of lower order. They can be obtained, however, by a variety of well-known methods from $\rho_{app}(x)$, p_N, and p_{N-1}.[15, 18, 19]

C. Spectral resolution of the full Green's function

We now propose to apply our knowledge of the quadrature generated by $H_0 + V_{app}$ to learn how to handle singular integrals by considering the spectral resolution of the Green's function[16]

$$g^P(E, r, r') = \frac{2}{\pi} P \int_0^\infty \frac{dE' \Psi^P(k', r)\Psi^P(k', r')}{k'[1 + \tan^2\delta(E')](E' - E)} \qquad (4.12)$$

when there are no bound states. The matrix elements in the basis ϕ_n are then

$$g^P_{nn'} = \frac{2}{\pi} P \int_0^\infty \frac{dE' R_n(k') R_{n'}(k')}{k'[1 + \tan^2\delta(E')](E' - E)} . \qquad (4.13)$$

Transforming the integration variable to x, introducing the weight function in numerator and denominator and subtracting an appropriate factor to simplify the singularity at $E' = E$, as we did in Eq. (3.11), yields

$$g^0_{nn'} = \frac{2X^{1/2}(x)}{\pi k} \int_{x(0)}^{x(\infty)} dx' \rho_{app}(x') \left(\frac{R_n(x') R_{n'}(x')}{X^{1/2}(x')\rho_{app}(x')(1 + \tan^2\delta(E'))} - \frac{R_n(x) R_{n'}(x)}{X^{1/2}(x)\rho_{app}(x)[1 + \tan^2\delta(E)]} \right) + \frac{2R_n(x) R_{n'}(x) P}{k[1 + \tan^2\delta(E)]\pi\rho_{app}} \int_{x(0)}^{x(\infty)} \frac{dx' \rho_{app}(x')}{x' - x} . \qquad (4.14)$$

when $n_>$, the greater of n and n', is larger than N, consideration of Eq. (4.10) for R_n and the remarks in Appendix A on the structure of R_n for $n \leq N - 1$ reveal that the integrand in the nonsingular integral above is $\rho_{app}(x)$ multiplied with a polynomial of degree $\leq 2n_> - 1$, and hence that a Gauss quadrature of degree $n_>$ will be exact.[15] With an eye toward comparing the result with the equally exact J-matrix expression, we perform this quadrature, whose abscissas lie at the zeros of $R_{n_>}(x')$, yielding

$$g^P_{nn'}(E) = \frac{2R_n(x) R_{n'}(x)}{k[1 + \tan^2\delta(E)]\pi\rho_{app}(x)} \times \left(P \int_{x(0)}^{x(\infty)} \frac{dx' \rho_{app}(x')}{x' - x} \sum_{j=1}^{n_>} \frac{w_j^{n_>}}{x_j^n - x} \right), \qquad (4.15)$$

where w_j^n is the Christoffel weight[15] appropriate to the quadrature of degree $n_>$ and P denotes the principle part of the given integral. Comparison with the exact J-matrix expression in Eq. (3.25b) implies

$$I_n(x) = \frac{R_n(x)}{\pi\rho_{app}(x)} \left(P \int_{x(0)}^{x(\infty)} \frac{dx' \rho_{app}(x')}{x' - x} - \sum_{j=1}^{n} \frac{w_j^n}{x_j^n - x} \right) \text{ for } n \geq N. \qquad (4.16)$$

Using Eq. (4.10) for $R_n(x)$, this means that $I_n(x)$ can be written as

$$I_n(x) = a_n \{X^{1/2}(x)\rho_{app}(x)[1 + \tan^2\delta(E)]\}^{1/2} q_n(x) , \qquad (4.17)$$

with $q_n(x)$ defined as

$$q_n(x)=\frac{P}{\pi\rho_{\rm app}(x)}\int_{x(0)}^{x(\infty)}\frac{dx'\,\rho_{\rm app}(x')p_n(x')}{x'-x}, \tag{4.18}$$

in close analogy with Eqs. (3.6) and (3.9)–(3.11) relating the c_n and s_n.

When $n_>$ is $\leq N-1$, the discussion in Appendix A shows that the integrand in the nonsingular integral in Eq. (4.14) for the Green's function is $\rho_{\rm app}(x')$ multiplied with a polynomial of degree $\leq 2N-3$, and hence a quadrature of degree N will be exact. With the help of Eq. (4.16), this yields

$$\mathcal{G}^P_{nn'}(E)=\frac{2X^{1/2}(x)}{\pi k}\times\sum_{j=1}^{N}\frac{\Gamma_{nj}\Gamma_{n'j}w_j k_{N-1}p_{N-1}(x_j)p'_N(x_j)}{(E_j-E)k_N h_{N-1}}+\frac{2R_n(x)R_{n'}(x)I_N(x)}{k(1+\tan^2\delta(E))R_N(x)}. \tag{4.19}$$

By expressing $R_n(x_j)$ in terms of $R_{N-1}(x_j)$ and dR_N/dx through Eq. (3.16b), the sum in Eq. (4.19) further simplifies with the help of Eq. (4.10) and the explicit forms of $x(E)$, a_n, and h_n in Table I to

$$\mathcal{G}^P_{nn'}(E)=\sum_{j=1}^{N}\frac{\Gamma_{nj}\Gamma_{n'j}w_j k_{N-1}p_{N-1}(x_j)p'_N(x_j)}{(E_j-E)k_N h_{N-1}}+\frac{2R_n(x)R_{n'}(x)I_N(x)}{k[1+\tan^2\delta(E)]R_N(x)}, \tag{4.20}$$

which is equivalent to the J-matrix result in Eq. (3.25b) if the weights obey the Christoffel formula (2.4) with $A_{N-1}=k_N/k_{N-1}$, in agreement with Eq. (2.2).

In addition, the J-matrix result (3.25b) can be seen to be equivalent to a quadrature representation of the Green's function in accordance with Eq. (2.7).

Expressing the standing wave normalized $R_n(x)$ as a matrix element with the outgoing or incoming wave-energy δ functional normalized eigenvector $|E\rangle$ as

$$\langle n|E\rangle\langle E|n'\rangle=\frac{2R_{n'}(x)R_{n'}(x)}{\pi k(1+\tan^2\delta)}, \tag{4.21}$$

and using Eqs. (4.10) and (4.17) for p_n and q_n allows us to write Eq. (4.19) as

$$\mathcal{G}^P_{nn'}(E)=\sum_{j=1}^{N}\frac{w_j}{\rho(x_j)}\left(\frac{dE}{dx}\right)_{x_j}\langle n|E(x_j)\rangle\langle E(x_j)|n'\rangle+\pi\langle n|E\rangle\langle E|n'\rangle q_N(x)/p_N(x). \tag{4.22}$$

Equating the first term above with the first term in the J-matrix result (3.25b) verifies the normalization relation expressed in Eq. (2.9), while the second term above gives a compact form to the dispersion correction term in Eq. (2.7). However, the J-matrix method improves on a quadrature in the first N basis functions to give a smooth approximation to all the matrix elements in a complete basis by incorporating the solutions of the H_0 Schrödinger equation shifted by δ in phase.

V. FREDHOLM DETERMINANT

Now we can apply our knowledge of the J-matrix quadrature to learn about the spectral density. This is best expressed in terms of the Fredholm determinant, or Jost function[16]

$$D(E)\equiv\det[(H_0-E)^{-1}(H-E)], \tag{5.1}$$

which is the ratio of a regular solution to the full Schrödinger equation, obeying the same boundary conditions as the free solution at $r=0$, to the physical wave function, regular at the origin and asymptotically equal in magnitude but shifted in phase from a free wave at large r.[16] The phase of the determinant is the negative of the phase shift and its magnitude gives the density of the full continuum states compared to the free states.[16]

In their article, Heller *et al.*[9] developed a smooth approximation to $D(E)$ with the quadrature generated by diagonalization of (H_0-E) in the basis set (2.11) for s waves and $z=0$ and with a correct treatment of the singular integral, on which ours in Sec. IV is modeled. Yamani and Reinhardt[10] extended the analysis to general angular momentum, both basis sets (2.11) and (2.13) and all z. We follow their approach here, with a slight modification which reveals a close connection with the J-matrix method and, when coupled with the results of Sec. IV, leads to a particularly simple form for $D(E)$ in terms of $\rho_{\rm app}(x)$.

Because the Fredholm determinant is analytic in the upper half of the complex k plane and $D(-k)=D(k)$, the real and imaginary parts are related by the dispersion relation[16]

$$\mathrm{Re}D(E)=1+\frac{P}{\pi}\int_0^\infty\frac{dE'\,\mathrm{Im}D(E')}{E'-E}. \tag{5.2}$$

Transforming first from E' to x', introducing the weight function, and then removing the singularity at $E'=E$ yields an expression equivalent to that of Heller and co-workers,[10]

$$\mathrm{Re}D(E)=1+\frac{X^{1/2}(x)}{\pi k}\times\int_{x(0)}^{x(\infty)}\left(\frac{dx'\rho_0(x')}{x'-x}\times\frac{k'\,\mathrm{Im}D(E')}{X^{1/2}(x')\rho_0(x')}-\frac{k\,\mathrm{Im}D(E)}{X^{1/2}(x)\rho_0(x)}\right)+\frac{\mathrm{Im}D(E)}{\pi\rho_0(x)}P\int_{x(0)}^{x(\infty)}\frac{\rho_0(x')dx'}{x'-x}. \tag{5.3}$$

On performing a quadrature of degree N, the quadrature of the second term in the first integral can be combined with the second principle-value integral and considerably simplified with the help of Eqs. (3.6), (3.9), and (3.11) to give

$$\mathrm{Re}D(E) \simeq 1 + \frac{X^{1/2}(x)}{\pi k} \sum_{j=1}^{N} \frac{{}^0w_j {}^0k_j \, \mathrm{Im}D({}^0E_j)}{\rho({}^0x_j) X^{1/2}({}^0x_j)({}^0x_j - x)} + \frac{\mathrm{Im}D(E) c_N(x)}{s_N(x)} . \tag{5.4}$$

Since the phase of $D(E)$ is $-\delta(E)$, it follows that

$$\mathrm{Im}D(E) = -\tan\delta(E)\,\mathrm{Re}D(E) , \tag{5.5}$$

allowing the second term in Eq. (5.4) to be combined with the right-hand side. Then, using Eq. (3.16a) to express $s_N + c_N \tan\delta$ as R_N and $\tan(E_j^0)$ as $R_N(x_j^0)/c_N(x_j^0)$ yields

$$\frac{\mathrm{Re}D(E) R_N(x)}{s_N(x)} \simeq 1 - \frac{X^{1/2}(x)}{\pi k} \times \sum_{j=1}^{N} \frac{{}^0w_j R_N({}^0x_j) {}^0k_j \, \mathrm{Re}D({}^0E_j)}{\rho({}^0x_j) c_N({}^0x_j) X^{1/2}({}^0x_j)({}^0x_j - x)} . \tag{5.6}$$

Further simplification can be introduced by expressing the weights in terms of Eq. (3.11) evaluated at $x = x_j^0$ and returning from x to the variable E.

$$\frac{\mathrm{Re}D(E) R_N(x)}{s_N(x)} \simeq 1 + \sum_{j=1}^{N} \frac{\mathrm{Re}D({}^0E_j) R_N({}^0x_j)}{(E - {}^0E_j) s_N'({}^0x_j)} \left(\frac{dE}{dx}\right)_{{}^0x_j} , \tag{5.7}$$

where the prime on s_N' indicates differentiation with with respect to x. Eq. (5.7) is now in the form of a quadrature of Eq. (5.2) without first removing the singularity, giving a rational fraction in E, expressed as a Laurent series of residues at its poles. Heller *et al.*[9] showed that this approximation is nothing more than Eq. (5.1) for $D(E)$ evaluated as the ratio of the determinants of the $N \times N$ matrix representations of $H - E$ and $H_0 - E$:

$$D_{\mathrm{quad}}(E) = \prod_{j=1}^{N} \frac{E - E_j}{E - {}^0E_j} , \tag{5.8}$$

which holds exactly for V truncated to the N-dimensional representation V_{app}. For the oscillator basis, where E is just a constant times x, this is clearly equivalent to

$$D_{\mathrm{quad}}(E) = p_N(x)/p_N^0(x) . \tag{5.9}$$

For the Slater basis (2.11), it is necessary to check that $R_N \to s_N$ as $E \to \infty$, or $x \to 1$, and hence that $p_N(1) = p_N^0(1)$, to show that Eq. (5.9) holds there as well.

Combining Eqs. (5.9) and (5.7) gives

$$\mathrm{Re}D(E) = s_N(x) p_N(x) / R_N(x) p_N^0(x) , \tag{5.10}$$

while a subsequent check of the integrand in the first integral in Eq. (5.3) reveals that the integrand was $\rho_0(x)$ times a polynomial of degree $2N - 2$, making the quadrature exact.

With the help of Eqs. (3.6) and (4.10) this can be simplified further to

$$\mathrm{Re}D(E) = \left(\frac{\rho_0(x)}{\rho_{\mathrm{app}}(x)[1 + \tan^2\delta(E)]}\right)^{1/2} , \tag{5.11}$$

or using Eq. (5.5), that

$$|D(E)|^2 = \rho_0(x)/\rho_{\mathrm{app}}(x) . \tag{5.12}$$

While something like this form is to be expected from the interpretation of the magnitude squared of the Fredholm determinant as a ratio of the density of states,[16] we find its simplicity particularly appealing.

VI. SPACING OF THE PSEUDOSTATES AND THE HELLER DERIVATIVE RULE

A. Introduction: Heller's conjecture

So far, in the analysis of the spectrum of H_0 by Heller, and co-workers[8,10] and in the above analysis for $H_0 + V$, knowledge of the exact continuum states in the special basis sets (2.11) and (2.13) was used in a comparison with the pseudostates to show the validity of the equivalent quadrature idea through explicit construction of the appropriate weight function and orthogonal polynomials. Extending equivalent quadrature to arbitrary L^2 bases demands a way of constructing the necessary quadrature parameters such as the normalization factor $w_j/\rho(x_j)dE/dx_j$ in Eqs. (2.9) and (4.22) and an interpolation of the dispersion correction factor q_n/p_n directly from the pseudostates. Although this task can be approached in terms of the classical moment problem with the Stieltjes imaging[11] technique, we will follow a conjecture of Heller[7,10] based on the spacing of the pseudostate eigenvalues.

In looking for a simple method of obtaining the normalization factor in Eq. (2.9) directly from the quadrature abscissas, Heller[7,10] found an interesting relation to hold for the Chebyschev polynomials,[15]

$$p_N(x) = \sin(n+1)\theta/\sin\theta , \tag{6.1}$$

where $x = \cos\theta$, which have the weight function $\rho(x) = \sin\theta$ on $x \in (-1, 1)$ and are the zeroth-order polynomials for the Slater basis (2.11) with $l = 0$ and $Z = 0$ in the J-matrix method.

Arranged in increasing order, the abscissas

are located at

$$x_j^{(n)} = -\cos\left(\frac{j+1}{n+1}\pi\right), \quad j = 1, 2, \ldots, n, \tag{6.2}$$

while the weights are given by Eq. (2.4) as

$$w_j^{(n)} = \frac{\pi}{n+1}\sin^2\left(\frac{j+1}{n+1}\pi\right). \tag{6.3}$$

Heller noted that if the abscissas in Eq. (6.2) are considered as a continuous function of their number as $x(\xi)$ with

$$x(j) = x_j, \tag{6.4}$$

then the derivative of x with respect to ξ at $\xi = j$,

$$\left.\frac{dx}{d\xi}\right|_j = \frac{\pi}{n+1}\sin\left(\frac{j+1}{n+1}\pi\right), \tag{6.5}$$

is related to the weights as

$$\left.\frac{dx}{d\xi}\right|_j = \frac{w_j^{(n)}}{\rho(x_j^n)}. \tag{6.6}$$

The same method works on the Chebyschev polynomials of the first kind[15] as well. Moreover, if we consider the energy eigenvalues as a function of this numbering parameter ξ, we obtain for $E_j = E(x_j)$

$$\left.\frac{dE}{d\xi}\right|_j = \frac{w_j^{(n)}}{\rho(x_j^{(n)})}\left(\frac{dE}{dx}\right)_{x_j^{(n)}}, \tag{6.7}$$

which is just the factor in Eq. (2.9) relating the continuum state of energy E_j to the corresponding pseudostate.

Heller then conjectured that Eq. (6.7) should hold for any Gauss quadrature. Although Yamani[10] demonstrated the validity of the conjecture for several known weight functions numerically and we found it to give results comparable to Stieltjes imaging[11] as the last step in solving the classical moment problem in a calculation of the total photodetachment cross section of H^-,[11] only the Chebyschev polynomials exhibit the closed relationship interpolating the abscissas as a function of their number as in Eq. (6.2), which made the proof straightforward. In fact, without the existence of such a unique interpolation, the rule conjectures about the drivative of a function known at n points and hence is not really precisely enough posed to be proved or disproved.

That Eq. (6.7) is plausible for any quadrature, however, can be seen from the following argument. Consider the quadrature of an integral of some function $f(x)$ obtained by introducing the weight function ρ in both numerator and denominator,

$$\int_a^b f(x)dx = \int_a^b f(x)\frac{\rho(x)}{\rho(x)}dx \simeq \sum_{j=1}^{n}\frac{f(x_j^{(n)})w_j^{(n)}}{\rho(x_j^{(n)})}. \tag{6.8}$$

On the other hand, changing variables in the integral from x to $\xi = j$ yields

$$\int_a^b f(x)dx = \int_{\xi(a)}^{\xi(b)} f(x)\frac{dx}{d\xi}d\xi \simeq \sum_{j=1}^{n} f(x_j)\left(\frac{dx}{d\xi}\right)_j. \tag{6.9}$$

Comparison of the two approximations in Eq. (6.8) and (6.9) suggests that the derivative rule must at least hold asymptotically for large n.

It was this thinking which led us to examine the large n behavior in looking for a natural interpolation function and hence to a provable formulation of the derivative rule for the classical orthogonal polynomials in terms of their large n behavior and that of the conjugate functions q_n. In Sec. VI B, we use the asymptotic form developed in Appendix B to carry out the proof on the p_n^0 of Eq. (3.4) for the J-matrix method for $z = 0$ as an example, reserving the parallel demonstration for $z \neq 0$ to Appendix B. An extension to the J-matrix polynomials, p_n, of Eq. (4.10) in Sec. VI C then reveals a particularly interesting relation between the relative spacing of the eigenvalues of H_0 and those of $H_0 + V$ and the scattering phase shift.

B. Derivative rule for the H_0 quadrature

The polynomials, p_n^0, given in Table I for H_0 in the oscillator basis and the Slater basis for $z = 0$ belong to the family of classical orthogonal polynomials.[15] In Appendix B, it is shown that for these classical polynomials $q_n^0 + ip_n^0$ can be written as

$$q_n^0 + ip_n^0 = \frac{\mathfrak{A}_n(x)e^{im\xi}}{(\rho_0 X^{1/2})^{1/2}}, \tag{6.10}$$

where ρ_0 and X are given in Table I and $\xi = \pi - \theta = \cos^{-1}(-x)$, $m = n + l + 1$ for the Slater case but $\xi = 2(x)^{1/2}$, $m = (n + 1 + l/2)^{1/2}$ for the oscillator case and $\mathfrak{A}_n$ approaches a constant in x with phase $(-\frac{1}{2}l\pi)$ for large n, if x is not too close to the endpoints. Splitting Eq. (6.10) into its real and imaginary parts yields for $p^0{}_n$ and $q^0{}_n$

$$p_n^0 = \frac{[\mathrm{Im}(\mathfrak{A}_n)\cos m\xi + \mathrm{Re}(\mathfrak{A}_n)\sin m\xi]}{(\rho_0 X^{1/2})^{1/2}}, \tag{6.11a}$$

$$q_n^0 = \frac{[\mathrm{Re}(\mathfrak{A}_n)\cos m\xi - \mathrm{Im}(\mathfrak{A}_n)\sin m\xi]}{(\rho_0 X^{1/2})^{1/2}}. \tag{6.11b}$$

It is easy to see that the zeroes of p_n^0 occur at the

solutions of the equation

$$\tan m\xi(x) = -\frac{\mathrm{Im}[\mathfrak{A}_n(x)]}{\mathrm{Re}[\mathfrak{A}_n(x)]} = -\tan\arg[\mathfrak{A}_n(x)], \qquad (6.12)$$

which means that for large n, where $\arg\mathfrak{A}_n \sim \frac{1}{2}l\pi$, the zeros become evenly spaced in the variable ζ.

Now a simple trick suffices to number the zeros in p_n^0 determined by Eq. (6.12). We introduce a function $\xi^0(x)$ into Eq. (6.12) as

$$\tan[m\zeta - \xi^0(x)\pi] = -\frac{\mathrm{Im}[\mathfrak{A}_n(x)]}{\mathrm{Re}[\mathfrak{A}_n(x)]}, \qquad (6.13)$$

such that when $\xi^0(x)$ is an integer, p_n^0 has a zero just as in Eq. (6.4). $\xi^0(x)$ should then increase monotonely from 1 to n as x increases from x_1 to x_n so as to keep the argument of $\tan[m\zeta(x) - \xi^0(x)\pi]$ in Eq. (6.13) within a constant range of width π. Naturally, there is a different function $\xi^0(x)$ for each n, but we suppress that dependence here.

Before showing that $\xi^0(x)$ so defined satisfies the derivative rule (6.6), it is useful to simplify Eq. (6.13) and thereby free the choice of $\xi^0(x)$ of any dependence on the asymptotic form for large n. Solving Eq. (6.13) for $\tan(\xi^0\pi)$ gives

$$\tan\xi^0(x)\pi = p_n^0(x)/q_n^0(x), \qquad (6.14)$$

making it clear why ξ^0 is an integer at each zero of p_n^0, and from the form of q_n^0 in Eq. (3.10), only at the zeros of p_n^0 for $x\epsilon(a,b)$.

The derivative rule (6.6) then follows from the differentiation of $\xi^0(x)$,

$$\pi\sec^2(\xi^0\pi)\frac{d\xi^0}{dx} = \frac{d\{p_n^0/q_n^0\}}{dx}, \qquad (6.15)$$

which, using $\sec^2\theta = 1 + \tan^2\theta$, becomes

$$\frac{d\xi^0}{dx} = \frac{[q_n^0 p_n'^0 - p_n^0 q_n'^0]}{[\pi(p_n^{0^2} + q_n^{0^2})]}. \qquad (6.16)$$

This can be evaluated at a zero of p_n^0 with the help of Eq. (3.11) for $q_n^0(x)$ as

$$\left.\frac{d\xi^0}{dx}\right|_{x=x_j} = \left.\frac{p_n'^0}{\pi q_n^0}\right|_{x=x_j} = \frac{\rho_0(x_j)}{w_j}, \qquad (6.17)$$

which is fully equivalent to the desired result (6.6).

Note that the validity of this derivative rule does not depend on the choice of weight function or any particular asymptotic form; it merely follows from the definitions of $\xi^0(x)$ in Eq. (6.14) and of the conjugate functions q_n^0 in Eqs. (3.10)–(3.11). In fact, one can argue that we have only found a function with the required value and derivative at each of n points, and have not really proved anything significant at all. We shall see below, however, that this choice of an interpolating function suggested by the asymptotic form of p_n^0 is a natural one with some desirable properties.

In particular for the classical orthogonal polynomials, we note in Appendix B that p_n^0 and q_n^0 satisfy the same second order differential equation such that their Wronskian has a simple form and allowing Eq. (6.16) to be rewritten as

$$\frac{d\xi^0}{dx} = \frac{W_n}{[\pi\rho_0 X(p_n^{0^2} + q_n^{0^2})]}, \qquad (6.18)$$

where W_n is a positive constant. Since ρ_0 and X are both positive throughout the interval of integration, $\xi^0(x)$ increases monotonely for $x\epsilon(a,b)$, and hence $\xi^0(x)$ and $x(\xi^0)$ are single valued. For large n and x not too near the endpoints, Eq. (6.18) gives the even spacing $d\xi^0/dx = m/\pi$ consistent with the asymptotic form of Eq. (6.11a).

As might be expected from the long range of the Coulomb potential, arguments about the asymptotic spacing must be modified for the Pollaczek polynomials. We discuss the appropriate modification in Appendix C, and turn now to the J-matrix polynomials p_n, developed for the full Hamiltonian in Sec. IV.

C. Derivative rule for the H quadrature

Combining Eqs. (3.16a), (3.24a), (4.10), and (4.17) for R_n and I_n with Eqs. (3.6) and (3.9) for s_n and c_n, the polynomials p_n and conjugate functions q_n for the full Hamiltonian can be written in terms of p_n^0 and q_n^0 for H_0 as

$$p_n = (\rho_0/\rho_{\mathrm{app}})^{1/2}[p_n^0\cos\delta + q_n^0\sin\delta], \qquad (6.19a)$$

$$q_n = (\rho_0/\rho_{\mathrm{app}})^{1/2}[q_n^0\cos\delta - p_n^0\sin\delta], \qquad (6.19b)$$

or equivalently

$$q_n \pm ip_n = (\rho_0/\rho_{\mathrm{app}})^{1/2}e^{\pm i\delta}(q_n^0 \pm ip_n^0) = D(E \mp i\epsilon)(q_n^0 \pm ip_n^0), \qquad (6.20)$$

using Eq. (5.12) for the Fredholm determinant. A comparison of Eq. (6.19a) with Eq. (6.11) reveals that the zeros of p_n are shifted by δ from those of p_n^0. Indeed, if we define a numbering parameter $\xi(x)$ for the zeros of p_n just as in Eq. (6.14) implicitly as

$$\tan(\xi(x)\pi) = p_n(x)/q_n(x). \qquad (6.21)$$

Equations (6.14) and (6.19) imply that

$$\tan[\xi(x)\pi] = \tan[\xi^0(x)\pi + \delta]. \qquad (6.22)$$

Clearly the same argument that led from Eq. (6.14) to (6.17) verifies the derivative rule for $\xi(x)$ as well. Furthermore, since at high energies the phase shift δ vanishes and the spectral density of the full Hamiltonian approaches that of H_0, and hence the arguments of the tangents in Eq. (6.22) coincide, we can write

$$\xi(x) = \xi^0(x) + \delta/\pi. \qquad (6.23)$$

Like Eq. (5.12) for the Fredholm determinant, expression (6.23) for the relative spacing of the eigenvalues of H and H_0 is so simple that it immediately reveals the nature of the finite L^2 representation of the continuum. Evidently, $\xi(x)\pi$ plays the role of a phase shift in the discrete representation, advancing by π as the energy passes through each pseudostate eigenvalue, just as the actual phase shift starts in accordance with Levinson's theorem at $n_b\pi$,[16] where n_b is the number of bound states. Then the actual phase shift is obtained by subtracting this pseudostate phase, $\xi(x)\pi$, from the phase, $\xi^0(x)\pi$, for H_0.

Equation (6.23) shows the correct qualitative behavior as $E \to 0$ for the extension to potentials with bound states as well. Since the zeros of the classical polynomials, p_n^0, lie within the interval (a, b) corresponding to positive energy, ξ^0 must vanish as $E \to 0$, and hence by Levinson's theorem[16] $[\delta(0) = n_b\pi]$ that ξ should go to the number of bound states as $E \to 0$. This is not quite correct, however, because the number of actual bound states of V_{app} is an upper bound to the number of negative energy pseudostates, which is what ξ really numbers. Hopefully, if n is large enough, all the bound states will be represented, but here is another aspect which must be investigated in the extension to stronger potentials.

The derivative of Eq. (6.23) with respect to the energy,

$$\frac{d\xi}{dE} = \frac{d\xi^0}{dE} + \frac{1}{\pi}\frac{d\delta}{dE} , \tag{6.24}$$

contains additional information about the adequacy of the finite basis in representing the details of the continuous spectrum. In the neighborhood of a resonance at E_r of width $\Gamma \simeq \pi/|d\delta/dE|_{E=E_r}$, the phase shift δ rises sharply through π,[16] meaning that the pseudostates must bunch near E_r. If the total number of basis functions is too small, there may not be enough pseudostates, making the calculated resonance wider than Γ. On the other hand, causality arguments limit the rate of decrease of the phase shift with respect to the momentum k to $d\delta/dk > -\mathfrak{D}$, where $\mathfrak{D}$ is the approximate size of the scatterer or the approximate range of the potential.[16] By Eq. (6.24), such a decrease can be described with $d\xi/dk$ still positive only if $d\xi^0/dk > \pi d$. By taking n large in Eq. (6.16) with the help of the asymptotic form of p_n^0 and q_n^0 in Eq. (6.11), this can be written as $m\zeta/dk > \mathfrak{D}$, while using the specific form of $\zeta(x)$ and $x(E)$ for the two basis sets then reduces the relation to $m > \frac{1}{2}\lambda\mathfrak{D}$, or that $2n$ must be larger than the variable in the basis sets (2.11) and (2.13) when r reaches out to the range $\mathfrak{D}$ of the potential.

VII. DISCUSSION

By knowing the exact wave functions from the J-matrix method, we were able to determine the weight function and polynomials orthogonal on it for the Gauss quadrature generated by the diagonalization of $H_0 + V_{\text{app}}$ in a Slater and an oscillator basis. It is now clear that the equivalent quadrature Fredholm determinant and J-matrix methods are essentially equivalent, yielding the same result from the same appropriate treatment of the potential and exact treatment of H_0. In addition, the simplicity of Eq. (5.12) for the magnitude of the Fredholm determinant and Eq. (6.23) for the phase shift emphasizes the usefulness of Gauss quadrature of the continuum as a theoretical concept as well as a numerical method. In considering only scattering by potentials too weak to have bound states, however, we have limited the possible applications too strongly. We will now outline how this and other restrictions can be lifted by future work.

Incorporating bound states into the quadrature scheme should present no insurmountable obstacles. Since bound states occur at poles[16] in the outgoing scattering wave function at positive imaginary k, we expect the coefficients of the outgoing wave, $R_n/(1 - i\tan\delta)$ to have singularities there. Heller[7] has shown this to be true, with the bound states of V_{app} located at the poles of $R_N/(1 - i\tan\delta)$, or at

$$\mathcal{G}_{N-1,N-1}J_{N-1,N}(c_N + is_N) + c_{N-1} + is_{N-1} = 0 . \tag{7.1}$$

Since at the bound-state energies the standing wave reduces to the bound-state function, this means that the singularity is entirely in the approach of $\tan\delta$ to i. A glance at Eq. (4.10) for R_n in terms of the polynomials p_n indicates that then $\rho_{\text{app}}(x)$ must have simple poles at the bound states, which in turn leads via Eq. (5.12) correctly to simple zeros in the Fredholm determinant.[16] The means that the weight function will have to be extended in domain to negative energies to include a sum of weight factors times δ functionals following the approach of Yamani and Reinhardt[10] in defining the attractive Coulomb Pollaczek weight function and polynomials to describe the Rydberg series. The quadrature generated by the diagonalization of $H_0 + V_{\text{app}}$ will then approximate a sum over perhaps infinitely many bound states and an integral over the continuum with a finite sum over pseudostates. The conditions under which this quadrature is exact and the treatment of the type of singularity which appears in the full Green's function and which leads to the dispersion relation between q_n and p_n in Eq. (4.18) will have to be investigated.

It is a valid criticism of the J-matrix method that although the Slater and oscillator basis sets (2.11) and (2.13) are convenient for calculation, fixing the scaling factor at one value for all n restricts the basis set too strongly, meaning that unworkably large basis sets will be needed to treat interesting systems. That a scattering calculation at all energies requires a global representation of the spectral density[20] and is thus less amenable to optimization of parameters than a bound-state calculation is only a partial rebuttal. A possible generalization to arbitrary basis sets might take the following form. One would start with the separate diagonalization of H and H_0 in the same N basis functions and then numerically interpolate the spacing of the eigenvalues to obtain monotonically increasing functions $\xi(E)$ and $\xi^0(E)$ analogous to those discussed in Sec. VI. Since in an arbitrary basis the more appropriate variable x is not known, or may not even exist, E is the most natural choice, with $\rho(E)\,dE$ playing the role of $\rho(x)\,dx$. Assuming they are generally applicable, Eq. (6.23) then gives the phase shift $\delta(E)$ as π times the difference of the spacing functions $\xi(E)$ and $\xi^0(E)$, while by Eq. (6.7) $d\xi/dE$ evaluated at an eigenvalue $E_j^{(N)}$ gives the factor $w_j^{(N)}/\rho(E_j^N)$, converting pseudostate into continuum matrix elements. With Eq. (6.14) this would allow an approximation to perturbations sums over a complete set of intermediate states such as for the full Green's function of the form

$$\langle i|\,\mathcal{G}^P(E)\,|f\rangle \simeq \sum_{j-i}^{N} \frac{\langle i|\psi_j\rangle\langle\psi_j|f\rangle}{E_j - E} + \frac{\langle i|E\rangle\langle E|f\rangle\pi}{\tan[\xi(E)\pi]}\,, \tag{7.2}$$

where $\langle i|E\rangle\langle E|f\rangle$ must be interpolated numerically from $\langle i|\psi_j\rangle\langle\psi_j|f\rangle$. This scheme appears promising because of its simplicity and its known validity in the special basis sets (2.11) and (2.13), but the several assumptions must be proved for general bases and special techniques developed to carry out the inherently tricky numerical differentiations to make it reliable.

Finally there remains the generalization to multichannel scattering. Evidently a two-dimensional quadrature is required to describe the scattering of a projectile from a target having a set of bound and continuum states. We applied this idea without detailed theoretical support to the two-electron photodetachment of H^- by treating one electron with the J-matrix method with $z=0$ and the second by equivalent quadrature with $z=1$ as a rough guess at the asymptotic conditions appropriate to a scattering theory of the three-body Coulomb system.[6] A proper treatment for short-range forces must be equivalent to the Fadeev formalism,[16] while no correct formulation is as yet known for three particles interacting with the Coulomb force. Perhaps the quadrature concept will show a way to approach this problem.

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APPENDIX A: VERIFICATION THAT THE p_n ARE POLYNOMIALS

Lemma 1. $p_N(x)R_n(x)/R_N(x) = \pi_{N-1}$ for $n \leq N-1$, where π_{N-1} is some polynomial of degree $\leq N-1$.

Proof: Using Eqs. (3.16b), (3.17), and (4.11)

$$\frac{p_N R_n}{R_N} = J_{N-1,N} \sum_{j=1}^{N} \frac{\Gamma_{nj}\Gamma_{N-1,j}}{E - E_j}\, k_N \prod_{j=1}^{N} (x - x_j)\,. \tag{A1}$$

Focusing on the oscillator basis and using the expression in Table I we find

$$\frac{p_N R_n}{R_N} = k_N \frac{\Gamma(N+l+\frac{3}{2})}{2\lambda\Gamma(N)} \sum_{j=1}^{N} \Gamma_{nj}\Gamma_{N-1j} \prod_{k\neq j}^{N} (x - x_k)\,. \tag{A2a}$$

This is clearly a polynomial of degree $\leq N-1$.

For the Slater basis, we obtain

$$\frac{p_N R_n}{R_N} = k_N \frac{\Gamma(N+2l+2)}{\lambda\Gamma(N)} \times \sum_{j=1}^{N} \Gamma_{nj}\Gamma_{N-1j}(1 - x_j) \prod_{k\neq j}^{N} (x - x_k)\,, \tag{A2b}$$

which is also clearly a π_{N-1}. Since $R_{N-1}(x)$ has the desired zeros, this means that Eq. (4.10) holds for p_{N-1} as well

Lemma 2. $R_n(x)/R_N(x) = \pi_{n-N}$ for $n \geq N$ Proof: Using Eq. (3.16a) for R_n and (3.18) for $\tan\delta$

$$R_n = \frac{J_{N-1,N}\tilde{\mathcal{G}}_{N-1,N-1}(s_n c_N - c_n s_N) + s_n c_{N-1} - c_n s_{N-1}}{J_{N-1,N}\tilde{\mathcal{G}}_{N-1,N-1}c_N + c_{N-1}}\,. \tag{A3}$$

The denominator in Eq. (A3) is easily expressed in terms of R_N by Eq. (3.19), and the numerator can be simplified with the help of Eq. (3.16a) for R_{N-1}, yielding

$$R_n = R_N T_{nN-1} - R_{N-1} T_{nN}\,, \tag{A4}$$

where

$$T_{nm} \equiv (2J_{N-1,N}/k)(c_n s_m - s_n c_m)\,. \tag{A5}$$

Clearly $T_{mm}=0$. Using the recursion relations for c_n and s_n (3.8) and (3.2) it is straightforward to show that $T_{m+1,m}(x)=J_{N-1,N}/J_{m+1,m}$, a constant (see Table I), and that

$$T_{n+1,m}=-\frac{J_{nm}T_{nm}}{J_{n+1,m}}-\frac{J_{n,n-1}T_{n-1,m}}{J_{n-1,n}}$$

$$=cxT_{nm}+c'T_{n-1,m}\,, \tag{A6}$$

where c and c' are constants (see Table I). Hence Eq. (A6) is a three-term recursion relation for the T_{nm} starting with a constant at $n=m+1$, or T_{nm} is a polynomial of degree $n-m-1$. Since R_N/R_{N-1} is linear in x from lemma 1, this means that R_n in Eq. (A4) is R_N times a polynomial of degree $(n-N)$.

APPENDIX B: PROPERTIES OF q_n FOR THE CLASSICAL AND POLLACZEK POLYNOMIALS

1. Classical orthogonal polynomials

The classical polynomials are special in that they obey the second-order differential equation

$$\frac{d(X\rho p_n')}{dx}+\lambda_n\rho p_n=0 \tag{B1}$$

and the Rodriguez formula

$$p_n=[1/(K_n\rho)]D^n(\rho X^n)\,, \tag{B2}$$

where λ_n and K_n are constants. There are really only two kinds: the Jacobi polynomials, for which Eq. (B1) is the hypergeometric equation, and the Laguerre polynomials, for which it is the confluent hypergeometric equation. The particular weight functions and other parameters for each, as well as for the Gegenbauer special case of the Jacobi polynomials of interest for the J-matrix method in the Slater basis (2.11), are listed in Table II.

It is straightforward to show the the conjugate functions $q_n(x)$ defined by

$$q_n(x)\equiv\frac{P}{\pi\rho(x)}\int_a^b\frac{dx'\rho(x')p_n(x')}{x'-x}\,, \tag{B3}$$

also satisfy the differential equation (B1), whereupon it follows that the Wronskian of q_n and p_n is of the form

$$q_np_n'-p_nq_n'=W_n/(\rho X)\,. \tag{B4}$$

(See Table II for the constant W_n.)

The general trend of the asymptotic behavior of the q_n and p_n also follows from the differential equation (B1), for the function $P_n(\xi)=\rho^{1/2}X^{1/4}p_n(x)$, where $\xi'(x)=X^{-1/2}$, satisfies the differential equation

$$P_n''(\xi)+[m^2-R(\xi)]P_n(\xi)=0 \tag{B5}$$

if p_n satisfies (B1). The specific values of ξ, the n-dependent parameter m, and $R(\xi)$ are given in Table II for each case. A look at these values reveals that for n large and x not too close to the endpoints, $m^2>|R(\xi)|^2$, and hence that P_n and similiary $\rho^{1/2}X^{1/4}q_n(x)$ approach linear combinations of $\cos(m\xi)$ and $\sin(m\xi)$. Incidentally, it is clear from Eqs. (3.6) and (3.9) that the s_n and c_n of the J-matrix method obey Eq. (B5).

Given the choice of m and ξ as the natural asymptotic parameters, the specific forms for p_n and q_n

TABLE II. Parameters for the classical orthogonal polynomials (Ref. 15). The weight function $\rho(x)$ and integration limits for the variable x are listed for the two major types of classical orthogonal polynomials, Jacobi and Laguerre, and for the Gegenbauer special case of the Jacobi polynomials. In addition, the parameters are given for expressing the polynomials in terms of the Rodriguez formula $p_n=(K_n\rho)^{-1}d^n(\rho X^n)/dx^n$ and for the simplified differential equation $P_n''(\xi)+[m^2-R(\xi)]P_n(\xi)=0$ satisfied by $P_n(\xi)=\rho^{1/2}X^{1/4}p_n(x)$ useful in determining the large n behavior of the polynomials. The Wronskian with a second solution of this equation is given by the constant W_n.

Polynomial	Jacobi	Gegenbauer	Laguerre
(a,b)	$(-1,1)$	$(-1,1)$	$(0,\infty)$
$\rho(x)$	$(1-x)^\alpha(1+x)^\beta$	$(1-x^2)^{2\lambda-1}$	$x^\alpha e^{-x}$
$X(x)$	$1-x^2$	$1-x^2$	x
$K(n)$	$(-2)^n n!$	$\frac{(-2)^n n!\Gamma(2\lambda)\Gamma(n+\lambda+1/2)}{\Gamma(\lambda+1/2)\Gamma(n+2\lambda)}$	$n!$
m	$n+(\alpha+\beta+1)/2$	$n+\lambda$	$[n+(\alpha+1)/2]^{1/2}$
ξ	$\cos^{-1}(-x)$	$\cos^{-1}(-x)$	$2(x)^{1/2}$
$R(\xi)$	$\frac{\alpha^2-1/4}{4\cos^2(\xi/2)}+\frac{\beta^2-1/4}{4\sin^2(\xi/2)}$	$\frac{\lambda(\lambda-1)}{\sin^2(\xi)}$	$\frac{\xi^2}{16}+\frac{\alpha^2-1/4}{\xi^2}$
W_n	$\frac{2^{\alpha+\beta+1}\Gamma(n+\alpha+1)\Gamma(n+\beta+1)}{\Gamma(n+1)\Gamma(n+\alpha+\beta+1)}$	$\frac{\pi 4^{1-\lambda}\Gamma(n+2\lambda)}{\Gamma(n+1)\Gamma^2(\lambda)}$	$\frac{\Gamma(n+\alpha+1)}{\Gamma(n+1)}$

TABLE III. Classical polynomials and conjugate functions. The classical polynomials $p_n(x)$ and their conjugate functions $\pi\rho q_n(x) = P\int dx'\,\rho(x')p_n(x')/(x'-x)$ and $f_n(x) = q_n + ip_n$ expressed in terms of hypergeometric and confluent hypergeometric functions. The weight function $\rho(x)$ and other parameters $\zeta(x)$, W_n; and m are listed in Table II. The large n behavior of the $f_n(x) = \mathfrak{A}_n(x)e^{im\zeta}/(\rho X^{1/2})^{1/2}$ is expressed in terms of the asymptotic limit of $\mathfrak{A}_n(x)$ as $n \to \infty$.

Polynomial	$p_n(x)$	$q_n(x)$
Jacobi	$P_n^{\alpha,\beta}(x) = \binom{n+\alpha}{\alpha} F[-n, n+\alpha+\beta+1; 1+\alpha; (1-x)/2]$	$\frac{-2^{\alpha+\beta}\Gamma(n+\alpha+1)F}{\pi\rho(x)\Gamma(n+\alpha+\beta+1)}\,[n+1, -n-\alpha-\beta; 1-\alpha; (1-x)/2] + \cot(\alpha\pi)p_n$
Gegenbauer	$C_n^{\lambda}(x) = \binom{n+2\lambda-1}{2\lambda-1} F[-n, n+2\lambda; 1/2+\lambda; (1-x)/2]$	$\frac{-\Gamma(\lambda-1/2)F}{\Gamma(\lambda)\{\pi\rho(x)\}^{1/2}}\,[n+1, -n-2\lambda+1; 3/2-\lambda; (1-x)/2] - \tan(\lambda\pi)p_n$
Laguerre	$L_n^{\alpha}(x) = \binom{n+\alpha}{\alpha}\Phi(-n; 1+\alpha; x)$	$\frac{\Gamma(\alpha)}{\pi x^{\alpha}}\Phi(-n-\alpha; 1-\alpha; x) - \cot(\alpha\pi)p_n$
	$f_n(x)$	$\mathfrak{A}_n(x)$ as $n \to \infty$
Jacobi	$\frac{-2^{n+\alpha+\beta+1}\Gamma(n+\alpha+1)\Gamma(n+\beta+1)}{\pi\rho(x)(x-1)^{n+1}\Gamma(2n+\alpha+\beta+2)} F[n+1, n+\alpha+1; 2n+\alpha+\beta+2; 2/(1-x)]$	$(-1)^n t^{(1/2-\beta)}(W_n/m)^{1/2}$
Gegenbauer	$\frac{(-1)^n e^{im\zeta - i(\lambda-1)\pi/2}}{2^{\lambda-1}(\rho X^{1/2})^{1/2}} \binom{m+\lambda-1}{\lambda-1} F[-\lambda+1, \lambda; m+1; 1/(1-e^{-2i\zeta})]$	$(-1)^n t^{(1-\lambda)}(W_n/m)^{1/2}$
Laguerre	$\frac{\Gamma(n+\alpha+1)(xe^{-i\pi})^{\alpha}}{\pi\rho(x)}\,\Psi(n+\alpha+1; 1+\alpha; xe^{-i\pi})$	$t^{(1/2-\alpha)}(W_n/m)^{1/2}$

follow from the integral representation of

$$f_n(z) \equiv \frac{1}{\pi\rho(z)} \int_a^b \frac{dx'\rho(x')p_n(x')}{(x'-z)}, \tag{B6}$$

where $f_n(x \pm i\epsilon) = q_n \pm ip_n$. Using the Rodriguez formula (B2), the integral can be integrated by parts n times to yield

$$f_n(z) = \frac{n!}{\pi K_n \rho(z)} \int_a^b \frac{dx'\rho(x')X(x')^n}{(x'-z)^{n+1}}, \tag{B7}$$

which is now in the form of the integral representation of a hypergeometric equation for the Jacobi case and a confluent hypergeometric function for the Laguerre, giving f_n in the form

$$f_n(x+i\epsilon) = \mathfrak{A}_n(x)e^{im\zeta}/(\rho X^{1/2})^{1/2}, \tag{B8}$$

and with the help of certain linear transformations, q_n and p_n as well. The particular functions f_n, q_n, and p_n for each case are listed in Table III, with the formula for $\mathfrak{A}_n$ for the Gegenbauer polynomials resulting from an additional quadratic transformation. When n is large, standard methods can be used to show that $\mathfrak{A}_n$ approaches the constants listed in Table III as well.

As a by-product, this development of the conjugate functions q_n extends the formulas for c_n of Yamani and Fishman[3] to noninteger l. By evaluating q_n in Table III for the Gegenbauer case for $l = \lambda + 1$ and the Laguerre case for $l = \alpha + \frac{1}{2}$ and using Eq. (3.9) for c_n, it follows that the factor $s_n \tan(\pi l)$ must be added to the formulas for c_n in Ref. 3 when l is not an integer.

2. *Pollaczek polynomials*

The Pollaczek polynomials[3,10,15,17] arise from the introduction of two extra parameters $\mathfrak{a}$ and $\mathfrak{b}$ into the three term recursion relation for the Gegenbauer polynomials so that

$$(n+1)p_{n+1} - 2[(n+\lambda+\mathfrak{a})x + \mathfrak{b}]p_n + (n+2\lambda-1)p_{n-1} = 0, \tag{B9}$$

starting with $p_0 = 1$ and $p_{-1} \equiv 0$. They are orthogonal on the weight function

$$\rho(x) = 2^{2\lambda-1}/\pi\, e^{(2\theta-\pi)t}(\sin\theta)^{2\lambda-1}\,|\Gamma(\lambda+it)|, \tag{B10}$$

where $t = (\mathfrak{a}\cos\theta + \mathfrak{b})/\sin\theta$ and $x = \cos\theta$, and are of interest in relation to the Coulomb Hamiltonian (2.14) with $\lambda = l+1$ and $\mathfrak{a} = -\mathfrak{b}$ such that $t = -z/k$.

Although they obey no differential equation, the p_n and be written in terms of hypergeometric functions as

$$p_n = \binom{n+2\lambda-1}{2\lambda-1} e^{in\theta}\,{}_2F_1(-n, \lambda+it; 2\lambda; 1-e^{2i\theta}). \tag{B11}$$

Using the definition of the conjugate functions q_n in Eq. (B3) or f_n in Eq. (B6) and considerable effort paralleling Szegö's proof of the orthogonality of the polynomials, it can be shown for $\mathfrak{a} > |\mathfrak{b}|$ that

$$f_n(x+i\epsilon) = q_n + ip_n = \mathfrak{C}_n(x) e^{im\zeta}/(\rho X^{1/2})^{1/2}, \quad \text{(B12)}$$

where $m = n+\lambda$,

$$\mathfrak{C}_n = (-1)^n \left(\frac{2}{\pi}\right)^{1/2} \frac{\Gamma(m+\lambda)}{|\Gamma(m+1-it)|} e^{-i(\lambda-1)\pi/2-\delta_p} \times {}_2F_1\left(-\lambda+1-it, \lambda+it;\ m+1-it;\ \frac{1}{1-e^{-2i\zeta}}\right) \quad \text{(B13)}$$

and

$$\delta_p = -t\ln(2\sin\zeta) + \arg\Gamma(m+1-it) - \arg\Gamma(\lambda-it). \quad \text{(B14)}$$

When n is large and x not too close to the endpoints -1 and 1, $\mathfrak{C}_n$ goes to a constant like the Gegenbauer polynomials, but with the additional phase $-\delta_p$.

Restricting our attention to $\lambda = l+1$ and $t = -z/k$, we can see the effect of this extra phase on the quadrature representation of the spectral density. The third term in Eq. (B14) contains what is generally known as the Coulomb phase shift,[16] while the first two terms must be involved in building up the divergent phase, $\ln(2kr)$,[16] in $S(r)$ in Eq. (3.1). For $z>0$, the eigenvalues are all pushed to higher energies by the repulsive Coulomb potential, while for $z<0$ the eignevalues are displaced in the other direction so strongly that a few are removed from the interval $(-1,1)$, consistent with the existence of bound states with an attractive Coulomb potential and with the failure of the proof of the orthogonality of the polynomials and of Eqs. (B12) and (B13) for $\mathfrak{a} < |\mathfrak{b}|$. That δ_p becomes infinite as $E \to 0$, corresponding to the infinite number of Coulomb bound states, while the number of bound pseudostates remains small, is another aspect of the representation of the bound states by pseudostates still be be explained.

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